What is claimed is:

1. A molecule or molecular complex comprising at least a portion of an *S. aureus* thioredoxin reductase or thioredoxin reductase-like FAD binding site, wherein the FAD binding site comprises the amino acids listed in Table 2, the FAD binding site being defined by a set of points having a root mean square deviation of less than about 1.1Å from points representing the backbone atoms of said amino acids as represented by the structure coordinates listed in Table 1.

2. The molecule or molecular complex of claim 1, wherein the FAD binding site comprises the amino acids listed in Table 3.

3. The molecule or molecular complex of claim 1, wherein the FAD binding site comprises the amino acids listed in Table 4.

4. A molecule or molecular complex comprising at least a portion of an *S. aureus* thioredoxin reductase or thioredoxin reductase-like NADPH binding site, wherein the NADPH binding site comprises Cys 135, Cys 138, and the amino acids listed in Table 5, the NADPH binding site being defined by a set of points having a root mean square deviation of less than about 0.8Å from points representing the backbone atoms of said amino acids as represented by the structure coordinates listed in Table 1.

5. The molecule or molecular complex of claim 4, wherein the NADPH binding site comprises Cys 135, Cys 138, and the amino acids listed in Table 6.

6. The molecule or molecular complex of claim 4, wherein the NADPH binding site comprises Cys 135, Cys 138, and the amino acids listed in Table 7.

7. A molecule or molecular complex that is structurally homologous to an *S. aureus* thioredoxin reductase molecule or molecular complex, wherein the *S. aureus* thioredoxin

reductase molecule or molecular complex is represented by at least a portion of the structure coordinates listed in Table 1.

8. A scalable three dimensional configuration of points, at least a portion of said points derived from structure coordinates of at least a portion of an *S. aureus* thioredoxin reductase molecule or molecular complex listed in Table 1 comprising at least one of a thioredoxin reductase or thioredoxin reductase-like FAD binding site or an NADPH binding site.

9. A scalable three dimensional configuration of points, wherein substantially all of said points are derived from structure coordinates of an *S. aureus* thioredoxin reductase molecule or molecular complex listed in Table 1.

10. The scalable three dimensional configuration of points of claim 8 wherein at least a portion of the points derived from the *S. aureus* thioredoxin reductase structure coordinates are derived from structure coordinates representing the locations of at least the backbone atoms of amino acids defining an *S. aureus* thioredoxin reductase FAD binding site, the FAD binding site comprising the amino acids listed in Table 2.

11. The scalable three dimensional configuration of points of claim 10 wherein the FAD binding site comprises the amino acids listed in Table 3.

12. The scalable three dimensional configuration of points of claim 10 wherein the FAD binding site comprises the amino acids listed in Table 4.

13. The scalable three dimensional configuration of points of claim 8 wherein at least a portion of the points derived from the *S. aureus* thioredoxin reductase structure coordinates are derived from structure coordinates representing the locations of at least the backbone atoms of amino acids defining an *S. aureus* thioredoxin reductase NADPH binding site, the NADPH binding site comprising Cys 135, Cys 138, and the amino acids listed in Table 5.

14. The scalable three dimensional configuration of points of claim 13 wherein the NADPH binding site comprises Cys 135, Cys 138, and the amino acids listed in Table 6.

15. The scalable three dimensional configuration of points of claim 13 wherein the NADPH binding site comprises Cys 135, Cys 138, and the amino acids listed in Table 7.

16. The scalable three dimensional configuration of points of claim 8 displayed as a holographic image, a stereodiagram, a model or a computer-displayed image.

17. A scalable three dimensional configuration of points, at least a portion of the points derived from structure coordinates of at least a portion of a molecule or a molecular complex that is structurally homologous to an *S. aureus* thioredoxin reductase molecule or molecular complex and comprises at least one of an *S. aureus* thioredoxin reductase or thioredoxin reductase-like FAD binding site or an NADPH binding site.

18. The scalable three-dimensional configuration of points of claim 17 displayed as a holographic image, a stereodiagram, a model or a computer-displayed image

19. A machine-readable data storage medium comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of at least one molecule or molecular complex selected from the group consisting of:

(i) a molecule or molecular complex comprising at least a portion of an *S. aureus* thioredoxin reductase or thioredoxin reductase-like FAD binding site comprising the amino acids listed in Table 2, the FAD binding site defined by a set of points having a root mean square deviation of less than about 1.1Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1; and

(ii) a molecule or molecular complex comprising at least a portion of an *S. aureus* thioredoxin reductase or thioredoxin reductase-like NADPH binding site comprising Cys 135, Cys 138, and the amino acids listed in Table 5, the NADPH binding site defined by a set of points having a root mean square deviation of less than about 0.8Å from points

representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1; and

(iii) a molecule or molecular complex that is structurally homologous to an *S. aureus* thioredoxin reductase molecule or molecular complex, wherein the *S. aureus* thioredoxin reductase molecule or molecular complex is represented by at least a portion of the structure coordinates listed in Table 1.

20. A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of machine readable data, using a machine programmed with instructions for using said first set of data and said second set of data, can determine at least a portion of the structure coordinates corresponding to the second set of machine readable data, wherein said first set of data comprises a Fourier transform of at least a portion of the structural coordinates for *S. aureus* thioredoxin reductase listed in Table 1; and said second set of data comprises an x-ray diffraction pattern of a molecule or molecular complex of unknown structure.

21. A method for obtaining structural information about a molecule or a molecular complex of unknown structure comprising:

crystallizing the molecule or molecular complex;

generating an x-ray diffraction pattern from the crystallized molecule or molecular complex;

applying at least a portion of the structure coordinates set forth Table 1 to the x-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown.

22. A method for homology modeling an *S. aureus* thioredoxin reductase homolog comprising:

aligning the amino acid sequence of an *S. aureus* thioredoxin reductase homolog with an amino acid sequence of *S. aureus* thioredoxin reductase and incorporating the sequence of the *S. aureus* thioredoxin reductase homolog into a model of *S. aureus* thioredoxin reductase

derived from structure coordinates set forth in Table 1 to yield a preliminary model of the *S. aureus* thioredoxin reductase homolog;

subjecting the preliminary model to energy minimization to yield an energy minimized model;

remodeling regions of the energy minimized model where stereochemistry restraints are violated to yield a final model of the *S. aureus* thioredoxin reductase homolog.

23. A computer-assisted method for identifying an inhibitor of *S. aureus* thioredoxin reductase activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* thioredoxin reductase or thioredoxin reductase-like FAD binding site, the FAD binding site comprising the amino acids listed in Table 2;

supplying the computer modeling application with a set of structure coordinates of a chemical entity; and

determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* thioredoxin reductase activity.

24. A computer-assisted method for identifying an inhibitor of *S. aureus* thioredoxin reductase activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* thioredoxin reductase or thioredoxin reductase-like NADPH binding site, the NADPH binding site comprising Cys 135, Cys 138, and the amino acids listed in Table 5;

supplying the computer modeling application with a set of structure coordinates of a chemical entity; and

determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule

or molecular complex is indicative of potential inhibition of *S. aureus* thioredoxin reductase activity.

25. The method of claim 23, wherein the FAD binding site comprises the amino acids listed in Table 2, the FAD binding site being defined by a set of points having a root mean square deviation of less than about 1.1Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

26. The method of claim 24, wherein the NADPH binding site comprises Cys 135, Cys 138, and the amino acids listed in Table 5, the NADPH binding site being defined by a set of points having a root mean square deviation of less than about 0.8Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

27. The method of claim 23 or 24, wherein determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex comprises performing a fitting operation between the chemical entity and a binding site of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between, or the interference with, the chemical entity and the binding site.

28. The method of claim 23 or 24 further comprising screening a library of chemical entities.

29. A computer-assisted method for designing an inhibitor of *S. aureus* thioredoxin reductase activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* thioredoxin reductase or thioredoxin reductase-like FAD binding site, the FAD binding site comprising the amino acids listed in Table 2;

supplying the computer modeling application with a set of structure coordinates for a chemical entity;

evaluating the potential binding or interfering interactions between the chemical entity and the FAD binding site of the molecule or molecular complex;

structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and

determining whether the modified chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to the molecule or molecular complex is indicative of potential inhibition of *S. aureus* thioredoxin reductase activity.

30. A computer-assisted method for designing an inhibitor of *S. aureus* thioredoxin reductase activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* thioredoxin reductase or thioredoxin reductase-like NADPH binding site, the NADPH binding site comprising Cys 135, Cys 138, and the amino acids listed in Table 5;

supplying the computer modeling application with a set of structure coordinates for a chemical entity;

evaluating the potential binding or interfering interactions between the chemical entity and the NADPH binding site of the molecule or molecular complex;

structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and

determining whether the modified chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to the molecule or molecular complex is indicative of potential inhibition of *S. aureus* thioredoxin reductase activity.

31. The method of claim 29, wherein the FAD binding site comprises the amino acids listed in Table 2, the FAD binding site being defined by a set of points having a root mean square deviation of less than about 1.1Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

32. The method of claim 30, wherein the NADPH binding site comprises Cys 135, Cys 138, and the amino acids listed in Table 5, the NADPH binding site being defined by a set of points having a root mean square deviation of less than about 0.8Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

33. The method of claim 29 or 30, wherein determining whether the modified chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex comprises performing a fitting operation between the chemical entity and a binding site of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between or interference with the chemical entity and the binding site.

34. The method of claim 29 or 30, wherein the set of structure coordinates for the chemical entity is obtained from a chemical fragment library

35. A computer-assisted method for designing an inhibitor of *S. aureus* thioredoxin reductase activity *de novo* comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* thioredoxin reductase or thioredoxin reductase-like FAD binding site, wherein the FAD binding site comprises the amino acids listed in Table 2;

computationally building a chemical entity represented by set of structure coordinates; and

determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* thioredoxin reductase activity.

36. A computer-assisted method for designing an inhibitor of *S. aureus* thioredoxin reductase activity *de novo* comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* thioredoxin reductase NADPH binding site, wherein the NADPH binding site comprises Cys 135, Cys 138, and the amino acids listed in Table 5;

computationally building a chemical entity represented by set of structure coordinates; and

determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* thioredoxin reductase activity.

37. The method of claim 35, wherein the FAD binding site comprises the amino acids listed in Table 2, the FAD binding site being defined by a set of points having a root mean square deviation of less than about 1.1Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

38. The method of claim 36, wherein the NADPH binding site comprises Cys 135, Cys 138, and the amino acids listed in Table 5, the NADPH binding site being defined by a set of points having a root mean square deviation of less than about 0.8Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

39. The method of claim 35 or 36, wherein determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex comprises performing a fitting operation between the chemical entity and a binding site of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between or interference with the chemical entity and the binding site.

40. The method of any of claims 23, 24, 29, 30, 35, or 36 further comprising providing the potential inhibitor, then assaying the potential inhibitor to determine whether it inhibits *S. aureus* thioredoxin reductase activity.

41. A method for making an inhibitor of *S. aureus* thioredoxin reductase activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield an inhibitor of *S. aureus* thioredoxin reductase activity, the chemical entity having been identified during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* thioredoxin reductase or thioredoxin reductase-like FAD binding site or an NADPH binding site; supplying the computer modeling application with a set of structure coordinates of a chemical entity; and determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex at a binding site, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* thioredoxin reductase activity.

42. A method for making an inhibitor of *S. aureus* thioredoxin reductase activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield an inhibitor of *S. aureus* thioredoxin reductase activity, the chemical entity having been designed during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* thioredoxin reductase or thioredoxin reductase-like FAD binding site or NADPH binding site; supplying the computer modeling application with a set of structure coordinates for a chemical entity; evaluating the potential binding interactions between the chemical entity and a binding site of the molecule or molecular complex; structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex at the binding site, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* thioredoxin reductase activity.

43. A method for making an inhibitor of *S. aureus* thioredoxin reductase activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield an inhibitor of *S. aureus* thioredoxin reductase activity, the chemical entity having been designed during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* thioredoxin reductase or thioredoxin reductase-like FAD binding site or an NADPH binding site; computationally building a chemical entity represented by set of structure coordinates; and determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex at a binding site, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* thioredoxin reductase activity.

44. An inhibitor of *S. aureus* thioredoxin reductase activity identified, designed or made according to the method of any of the claims 23, 24, 29, 30, 35, 36, 41, 42, or 43.

45. A composition comprising an inhibitor of *S. aureus* thioredoxin reductase activity identified, designed or made according to the method of any of claims 23, 24, 29, 30, 35, 36, 41, 42, or 43.

46. A pharmaceutical composition comprising an inhibitor of *S. aureus* thioredoxin reductase activity identified or designed according to the method of any of claims 23, 24, 29, 30, 35, 36, 41, 42, or 43 or a salt thereof, and pharmaceutically acceptable carrier.

47. A method for crystallizing an *S. aureus* thioredoxin reductase molecule or molecular complex comprising:

preparing purified *S. aureus* thioredoxin reductase at a concentration of about 1 mg/ml to about 50 mg/ml; and

crystallizing *S. aureus* thioredoxin reductase from a solution at a pH of about 6 to about 10 and comprising about 0 wt. % to about 40 wt. % DMSO and about 100 mM to about 6 M sodium formate.

48. A crystal of *S. aureus* thioredoxin reductase.

49. The crystal of claim 48 having the tetragonal space group symmetry $P4_32_12$.

50. The crystal of claim 48 comprising a unit cell having dimensions a, b, and c; wherein a is about 70Å to about 110Å, b is about 70Å to about 110Å, c is about 160Å to about 220Å, and $\alpha = \beta = \gamma = 90°$.

51. The crystal of claim 48 comprising atoms arranged in a spatial relationship represented by the structure coordinates listed in Table 1.

52. The crystal of claim 48 wherein thioredoxin reductase has amino acid sequence SEQ ID NO:1.

53. The crystal of claim 48 wherein thioredoxin reductase amino acid sequence SEQ ID NO:1, except that at least one methionine is replaced with selenomethionine.